AA11: Thermal Infrared Imaging Spectroscopy
IGARSS '98
Seattle, July 6-10, 1998

Surface Emissivity and Temperature Retrieval for a Hyperspectral Sensor

Christoph C. Borel
Space and Remote Sensing Sciences Group, NIS-2, MS C323,
Los Alamos National Laboratory, Los Alamos, NM 87545, USA,
E-mail : cborel@lanl.gov

Content:

- Introduction
- Synthetic Hypercube Generation
- A Temperature-Emissivity Separation (TES) algorithm
- Atmospheric Effects
- IR signature of gas plumes
- SEBASS data analysis for SO_2 and SF_6
- Conclusions

Introduction

Problem of Temperature-Emissivity Separation (TES):

Given are N spectral measurements of radiance and wanted are $N+1$ unknowns (N emissivities and one temperature) [Realmuto, 1990].

If atmosphere present we also need: $3N$ unknowns

- N spectral transmissions $T(\lambda_i)$,
- N up-welling path radiances $L_{path\uparrow(\lambda_i)}$, and
- N down-welling path radiances $L_{path\downarrow}(\lambda_i)$.

Previous Methods: (for multi-spectral case)

- Assumed channel 6 emittance model: Kahle et al., 1980,
- Emissivity Spectrum Normalization (ESN): Realmuto, 1990,
- Thermal log and alpha residual: Hook et al., 1992 and
- Mean-Maximum Difference (MMD): Matsunaga, 1993.

Hyperspectral Thermal Sensors:

$\Rightarrow$ Potential to separate emissivity, temperature and atmosphere using many channels (> 100) in TIR (8-12 μm).

Simple Observation:

A typical emissivity spectrum is rather smooth compared to spectral features introduced by gases in the atmosphere.

Idea:

Devise an adaptive solution technique to retrieve emissivity spectra ε_i based on spectral smoothness.

Note:

Similar approaches by:

-
-
-

Synthetic Hypercube Generation

Why synthetic data?

1. Can compare the retrieved emissivity to the truth.
2. Can assume that the sensor's spectral and radiometric performance is optimal.
3. Can perform sensitivity studies by assuming errors in the sensors performance and modeling of the atmosphere which are useful in:
   (a) Determining the retrieval errors for actual sensors
   (b) Come up with sensor specifications (e.g. SNR and spectral resolution) to meet a certain performance goal.

Geometry Model:

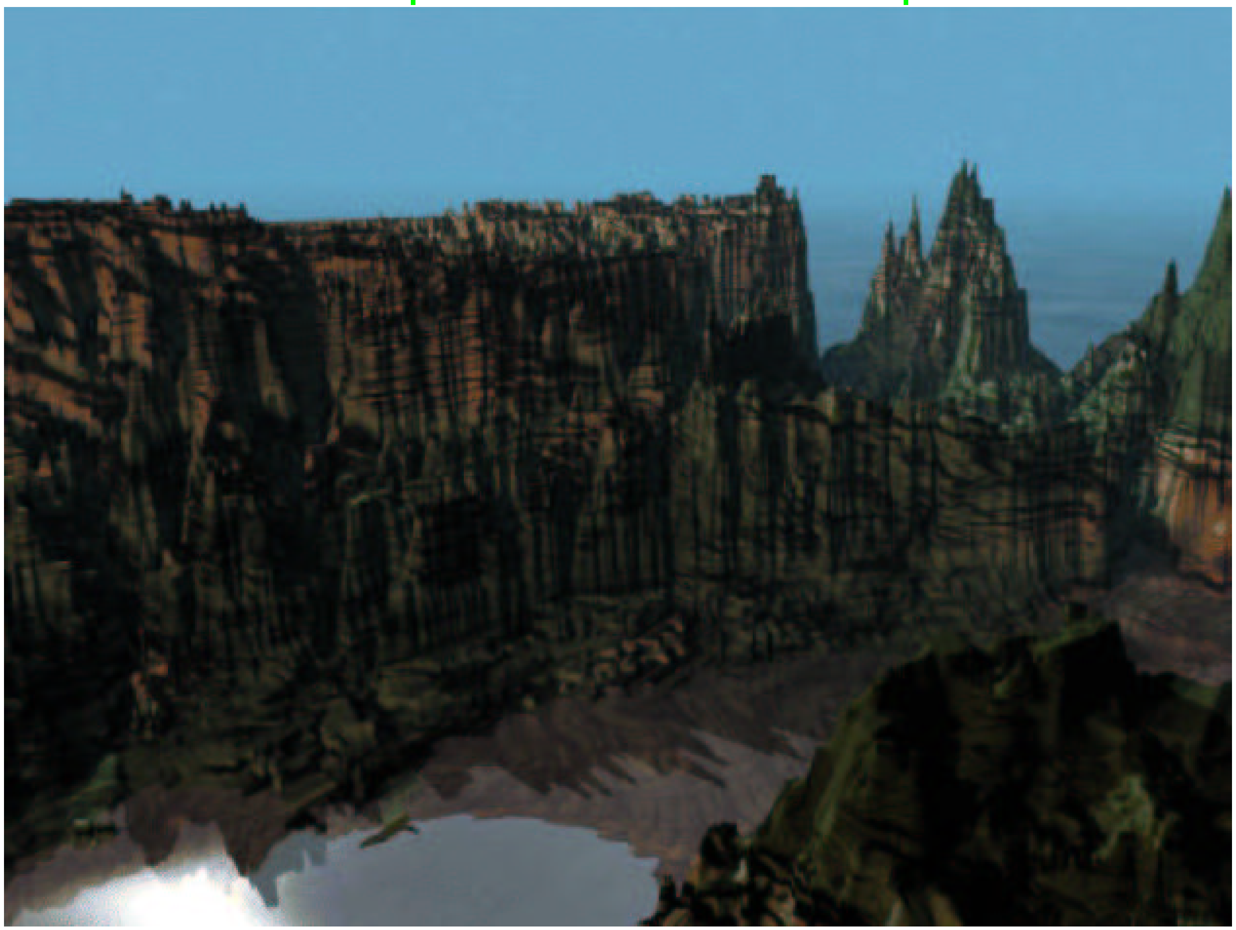
AC3D [Author: Andy Colebourne, andy@comp.lancs.ac.uk]

- Generate objects using graphics primitives (polygons, spheres, cones, ...)
- Easy to use, free.
- Generates output files for raytracer POV (and others: Dive, Massive, VRML, RenderMan).

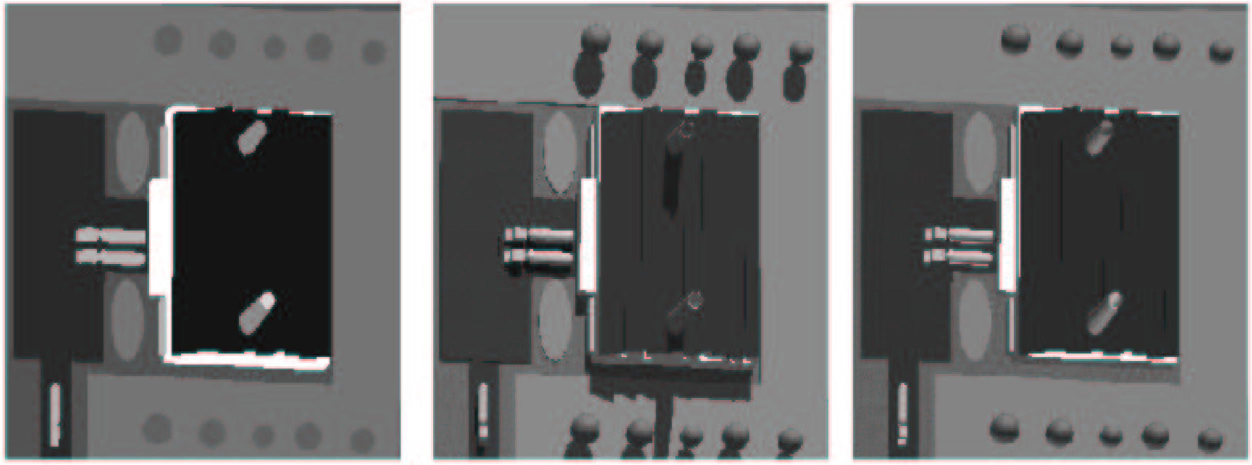
Renderer:

Persistence of Vision (POV) Raytracer [http://www.povray.org]

Example of a fractal landscape



Example of POV Ray runs



Material Map M(x,y) Shade(x,y) No_Shade(x,y)

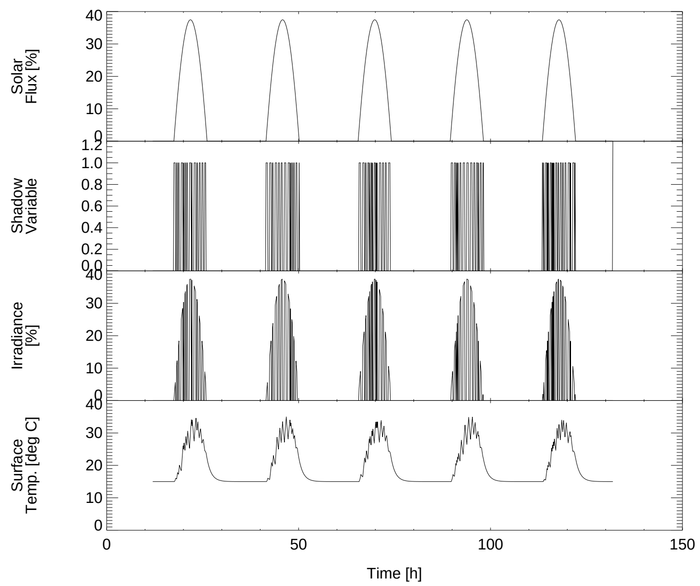
- High level description of complex scenes possible
- High quality rendering possible including Radiosity
- Free and runs on many platforms (UNIX, MAC and PC)

Ground leaving radiance:

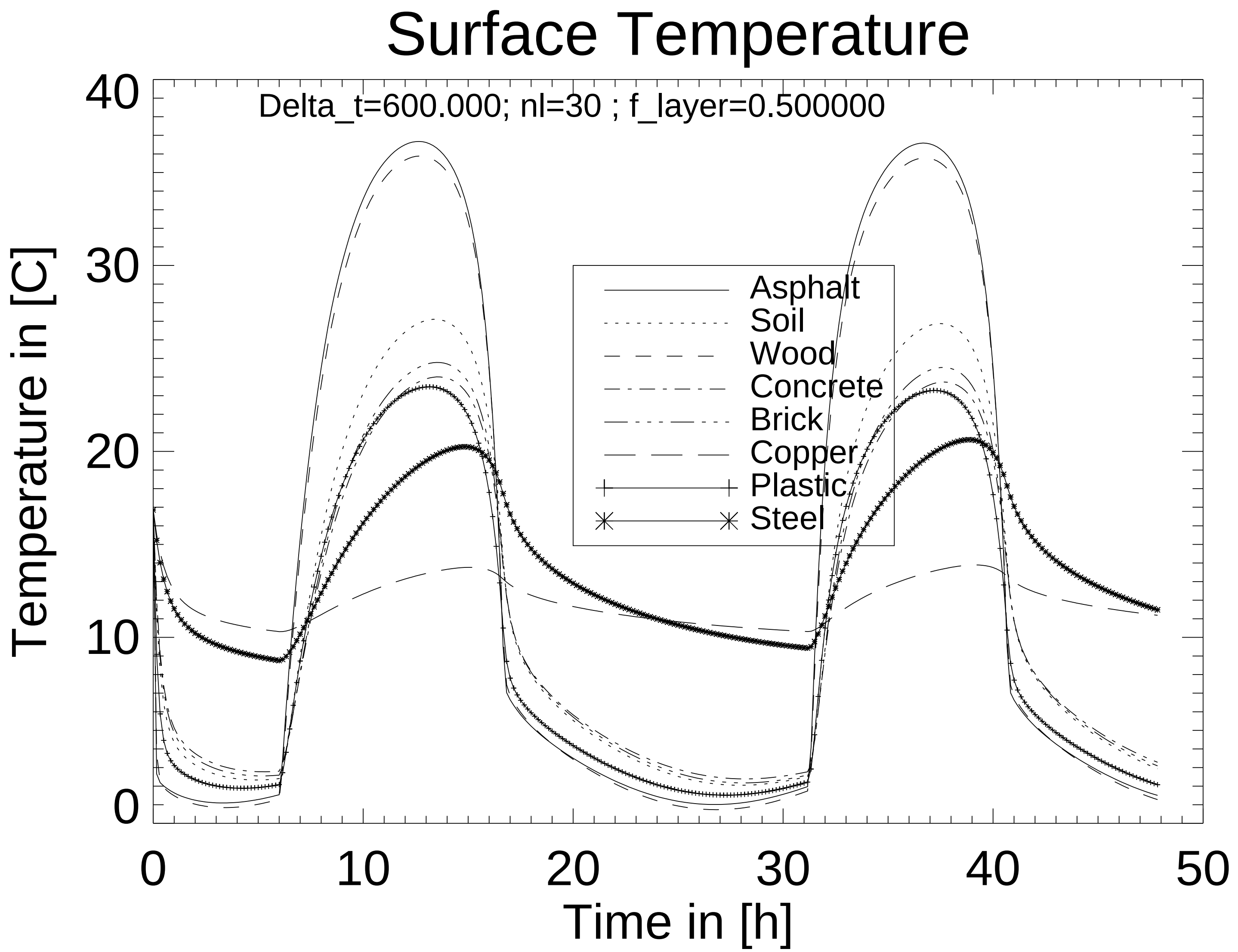
$$L_{ground}(\lambda, x, y) = \varepsilon(\lambda, M(x,y)B(\lambda, T(x, y, M(x,y)))$$

Thermal Model Features:

- 3 seasons (winter, spring and summer) give average and variance of day/night temperatures for grass, concrete, soil and vegetation. [P. Jacobs, 1996].
- Calculate normalize computed diurnal cycles of solar irradiance
  IDL routine zensun.pro in package esrgidl3.4 by Paul Ricchiazzi, Earth Space Research Group, UCSB, $http://skua.crseo.ucsb.edu/esrg.html$
- Surfaces retain heat using a time constant.
- Result is a ground temperature image $T_{ground}(x, y, t)$.

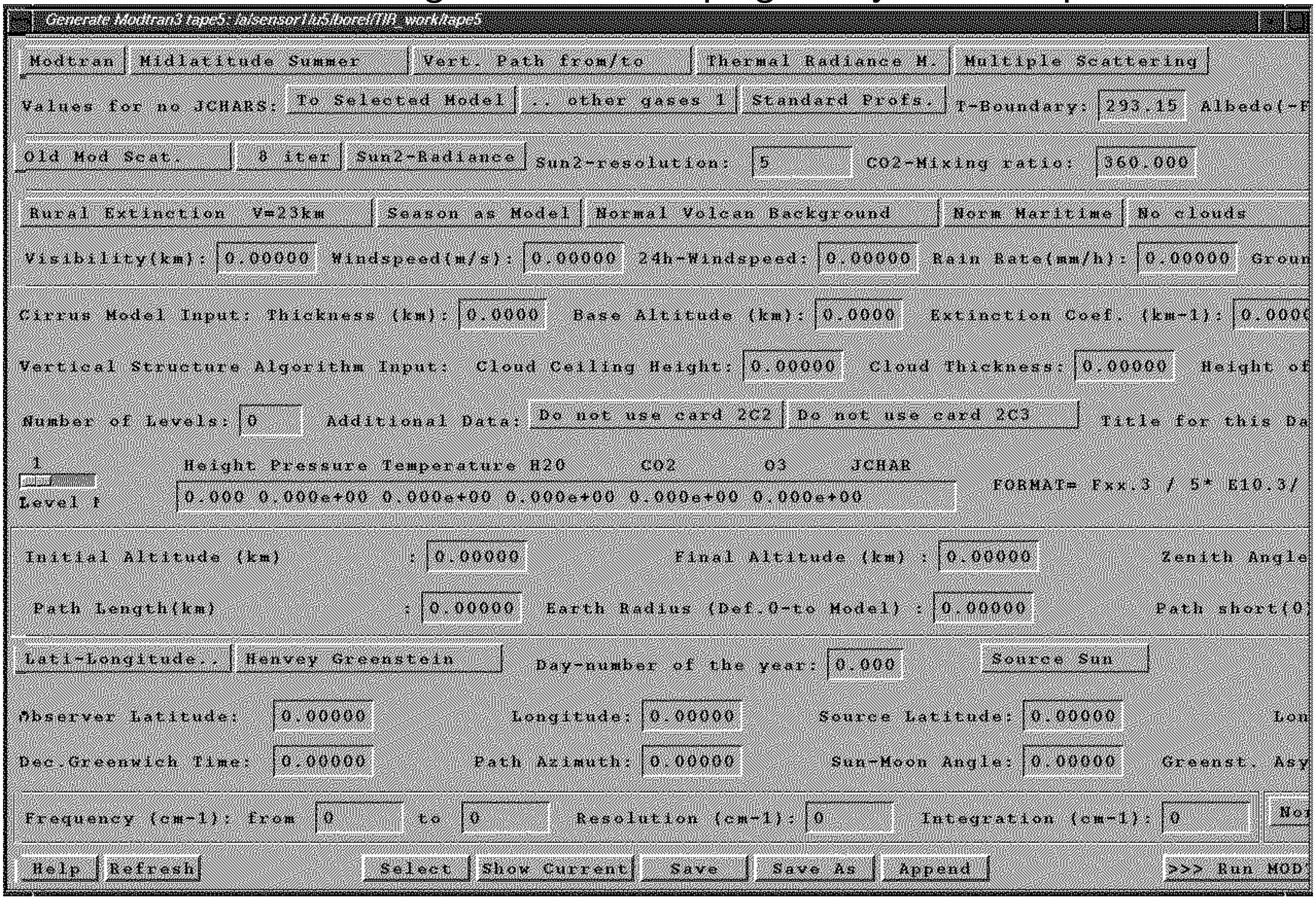


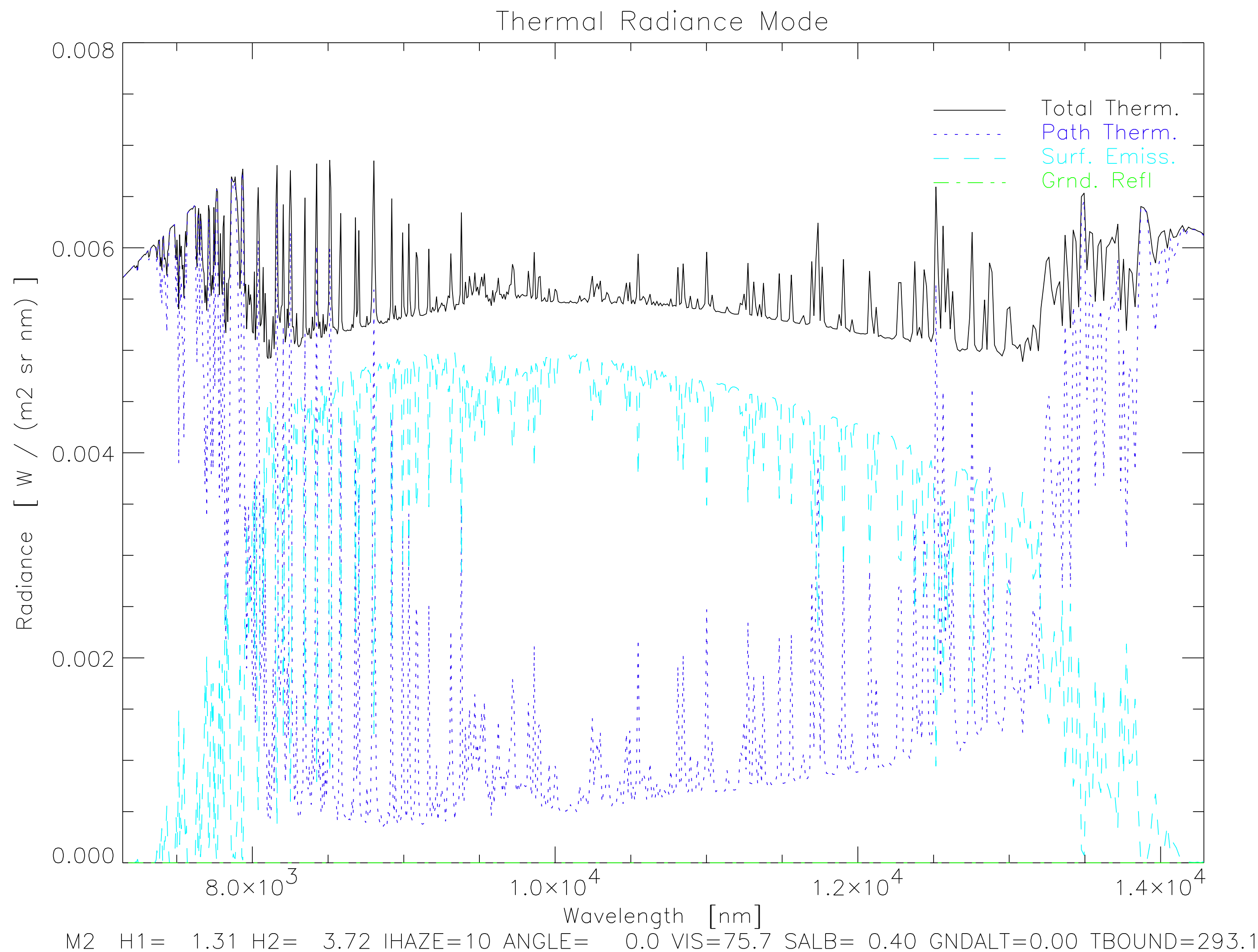
1-D thermal model results for various surface types



Atmospheric Model

Run MODTRAN 3 using Xmodcon IDL program by D. Schlaepfer




Thermal Radiance Mode
Total Therm.
Path Therm.
Surf. Emiss.
Grnd. Refl
0.008
0.006
0.004
0.002
0.000
Radiance [W / (m2 sr nm)]
8.0×10^3
1.0×10^4
1.2×10^4
1.4×10^4
Wavelength [nm]
M2 H1= 1.31 H2= 3.72 IHAZE=10 ANGLE= 0.0 VIS=75.7 SALB= 0.40 GNDALT=0.00 TBOUND=293.1

Data cube Generation

Radiance image cube:

$$L_{total}(x, y, \lambda) = L_{ground}(x, y, \lambda) + L_{path\uparrow}(\lambda) + L_{reflected}(x, y, \lambda) \tag{1}$$

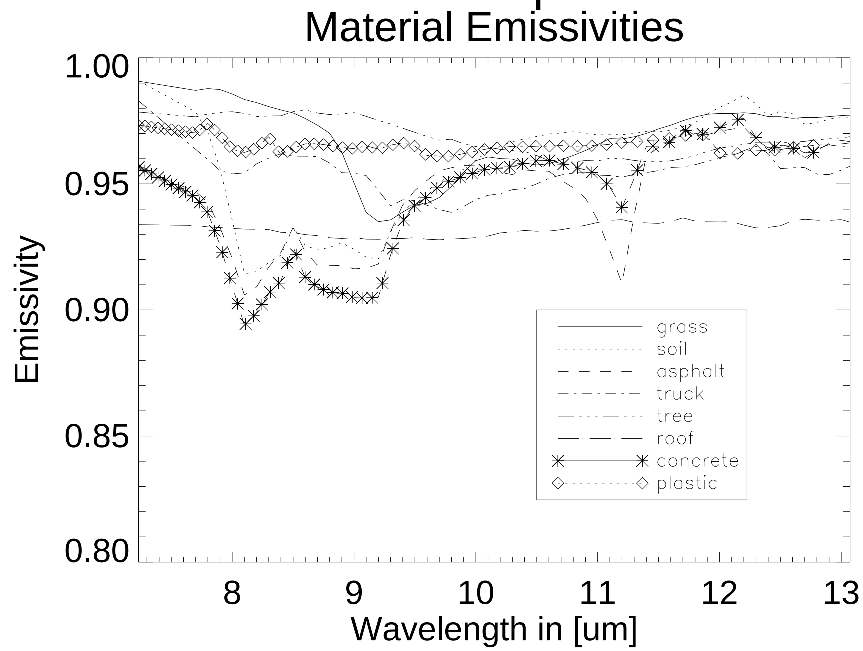
where:

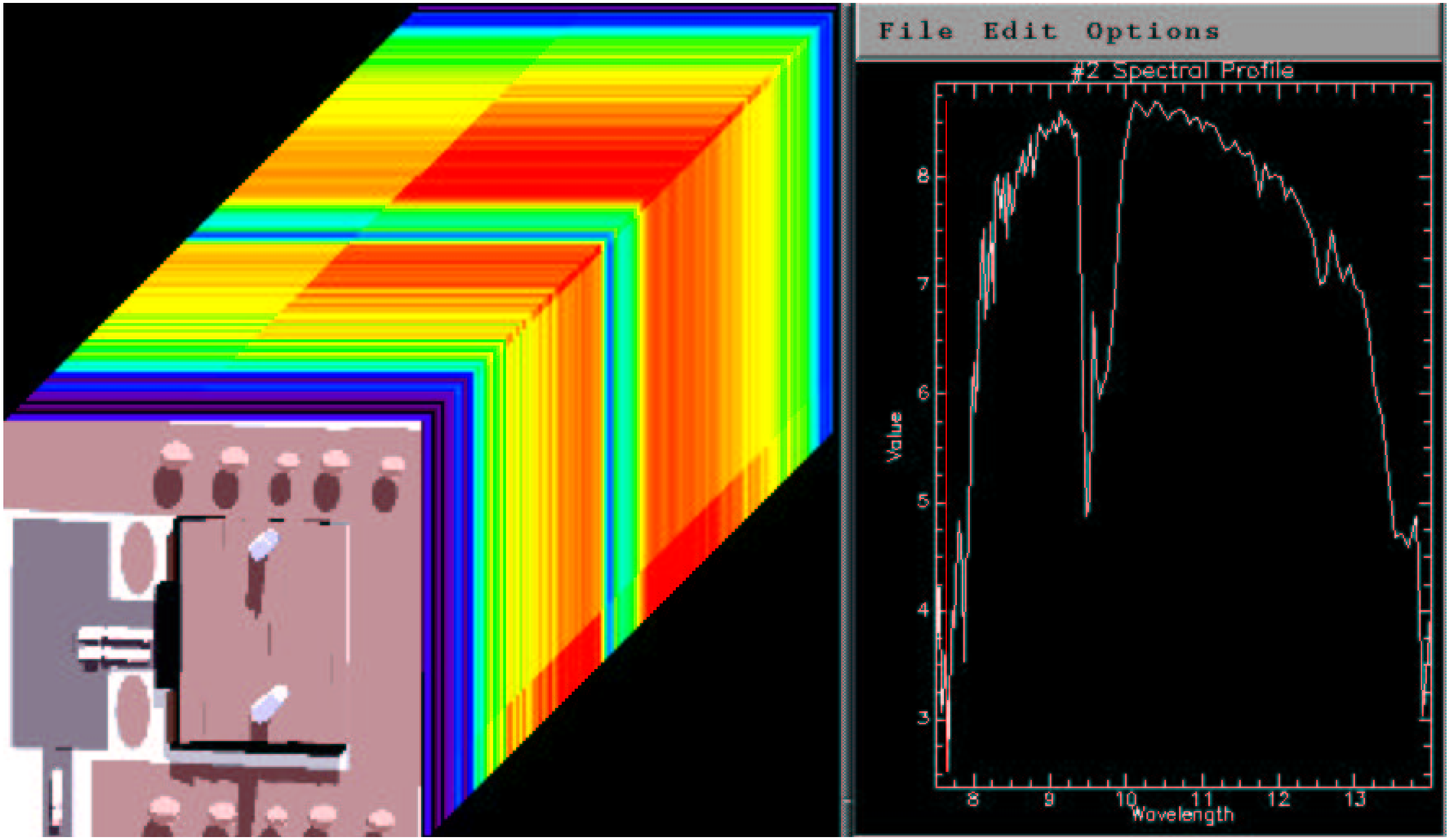
$$L_{ground}(x, y, \lambda) = \varepsilon(x, y, \lambda) B(\lambda, T_{ground}(x, y)) \tau_{atmo}(\lambda)$$

, and

$$L_{reflected}(x, y, \lambda) = L_{path\downarrow}(\lambda)[1 - \varepsilon(x, y, \lambda)] \tau_{atmo}(\lambda), \tag{2}$$

where $B(\lambda, T)$ is the Planck function for the spectral radiance in $[W/(cm^2 ster\, \mu m)]$.





Timing:

The generation takes about 30 sec for a $N_x x N_y x N_{chan} = 128x128x128$ ($5cm^{-1}$ sampling) cube and 8 min for a 320x320x751 ($1cm^{-1}$ sampling) cube on a SGI Indigo2 with a R8000 64-bit processor running at 75 MHz.

Adaptive Spectrally Smooth E-T Retrieval (ASSETR)

Observation:

Infrared spectra of solids are much smoother than are thermal-infrared spectra of gases.

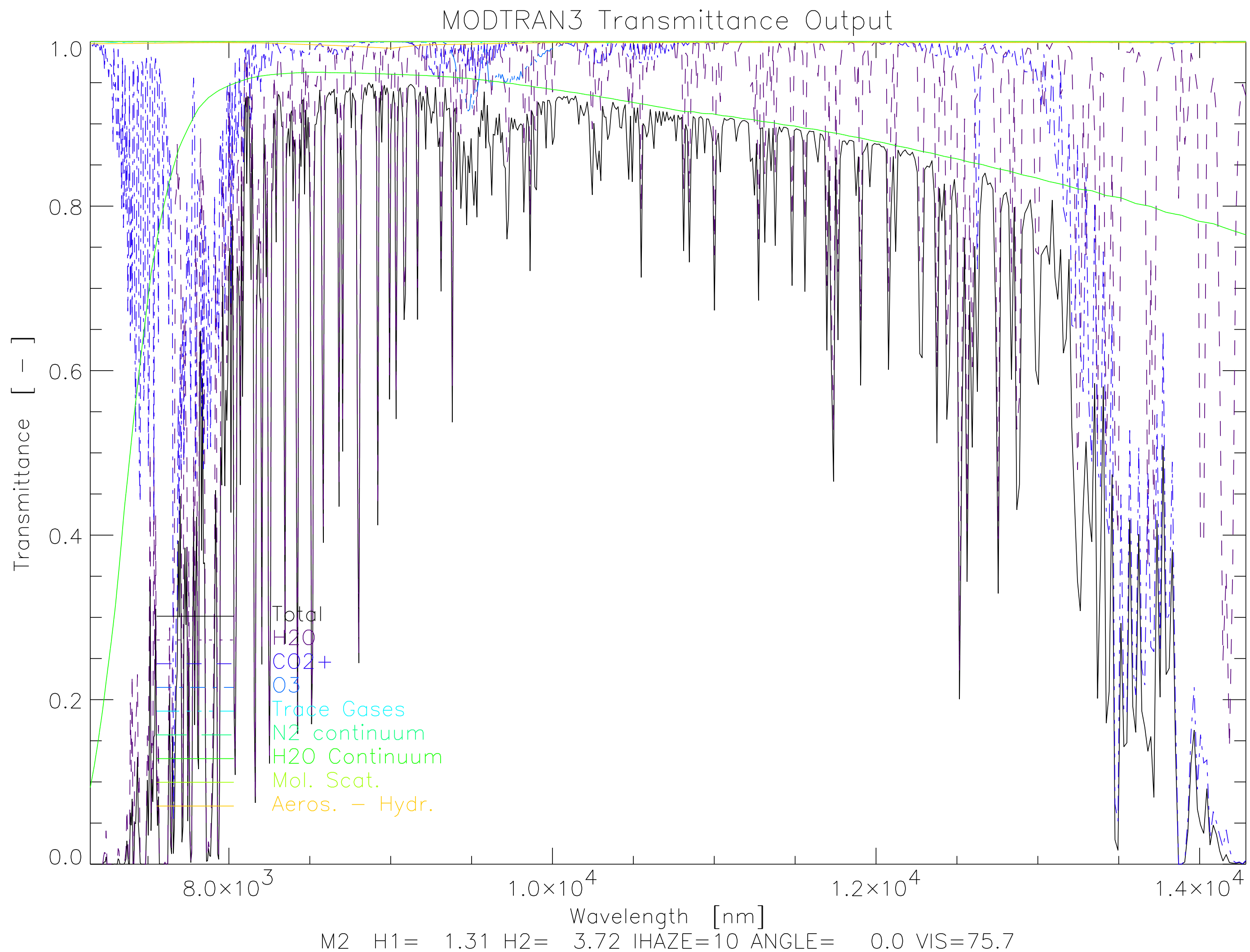
Why?

- Spectral features of solids tend to be fairly wide, whereas those in a gas tend to be more narrow.
- The width of a given spectral feature is inversely proportional to the lifetime of the transition which created it – short lifetimes give wide features whereas long lifetimes create narrow features.
  - Solid: molecules are bound together $\Rightarrow$ coupled, highly complex, vibrational system $\Rightarrow$ Wide bands
  - Gas: individual molecules are isolated and simple $\Rightarrow$ less phenomena can disrupt an excited state $\Rightarrow$ longer lifetimes and narrower spectral features.

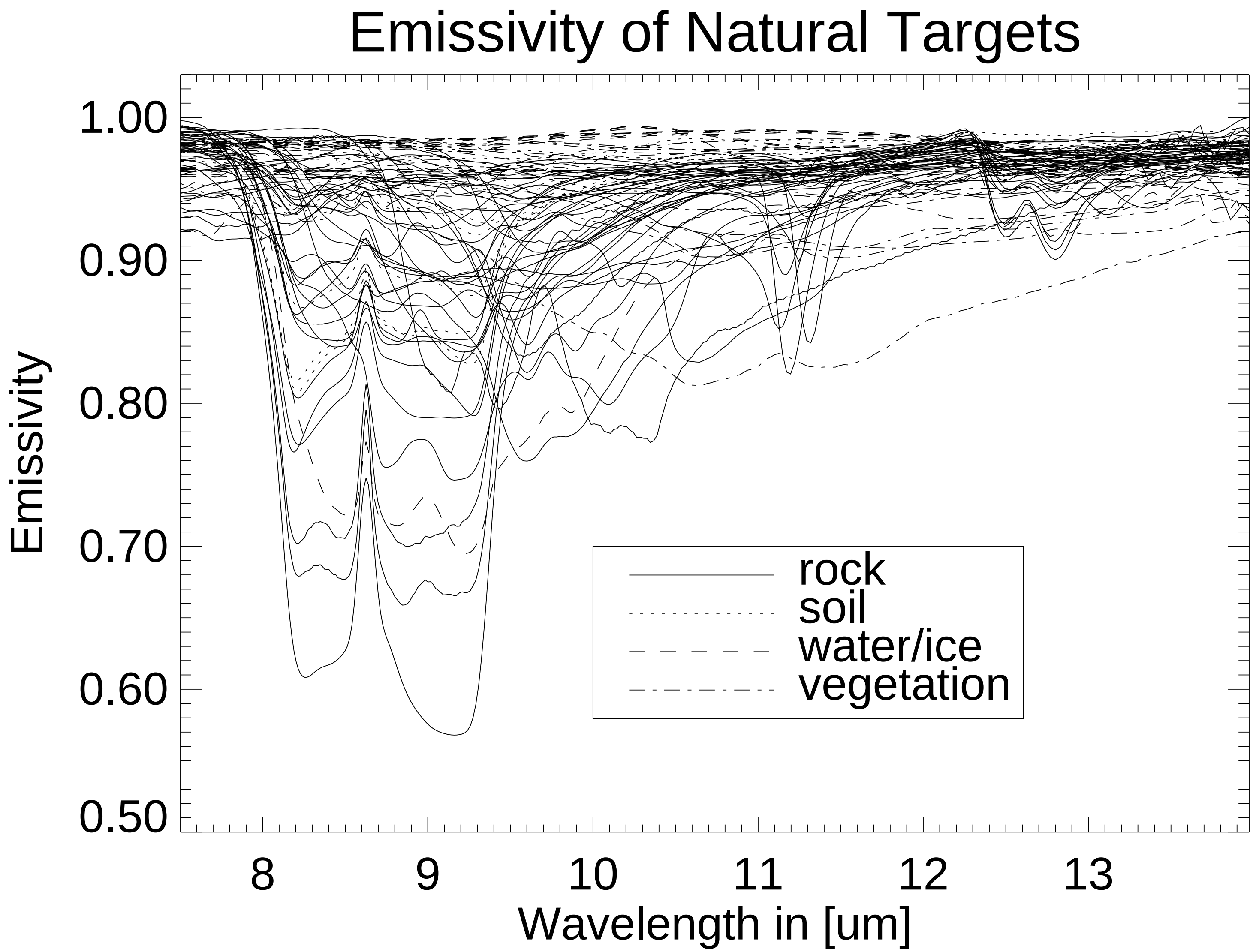
Experiment to Quantify Spectral Smoothness

Data sources:

- Transmission of the atmosphere using MODTRAN 3.



- Spectral libraries provided by Salisbury et al . (1992) for natural (rocks, soils, water/ice and vegetation) surfaces.



Measure of smoothness: Decorrelation wavenumber

Autocorrelation function $P_x(L)$ of a sample population x as a function of lag L:

$$P_x(L) = P_x(L) = \frac{\Sigma_{k=0}^{N-L-1}(x_k - \overline{x})(x_{k+L} - \overline{x})}{\Sigma_{k=0}^{N-1}(x_k - \overline{x})^2}. \tag{3}$$

Given the first few samples of $P_x(L), L = 0, 1, ..., L_{max}$ we calculate the average decorrelation wavenumber D_ν for a range of wavenumbers from L_{min} to L_{max} as:

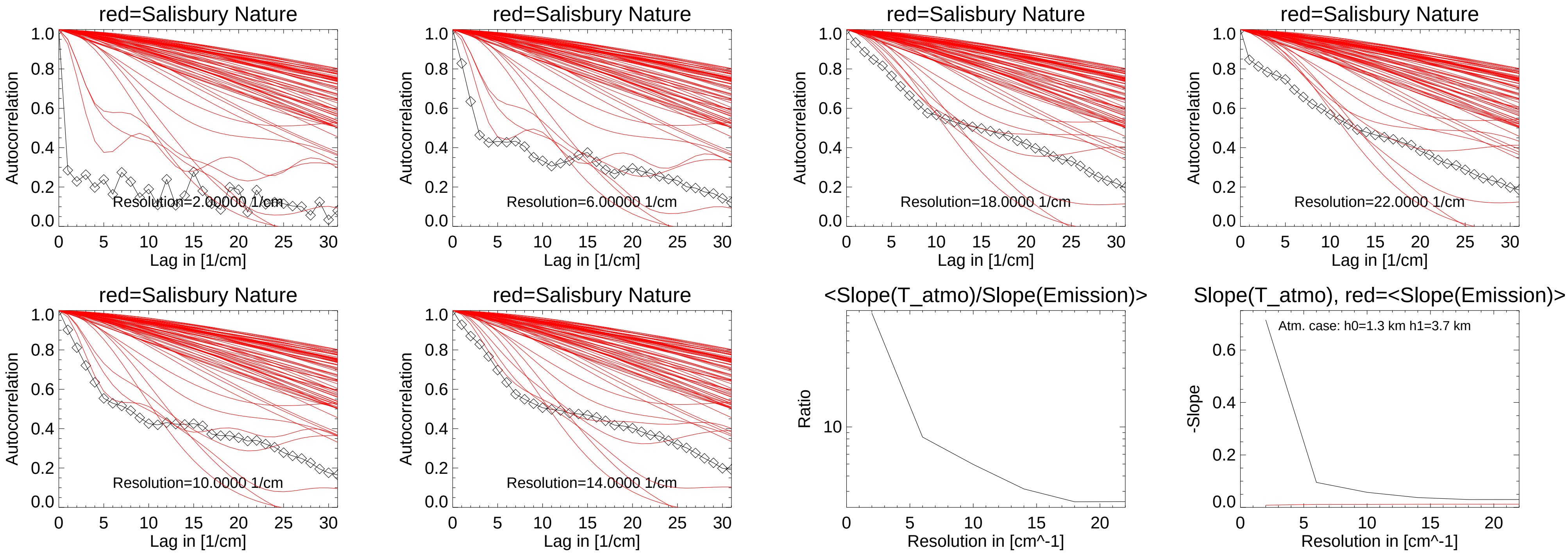
$$D_\nu = \frac{1}{L_{max} - L_{min} + 1} \sum_{L=L_{min},...,L_{max}} \frac{L}{P_x(0) - P_x(L)}. \tag{4}$$

Dependence on spectral resolution:

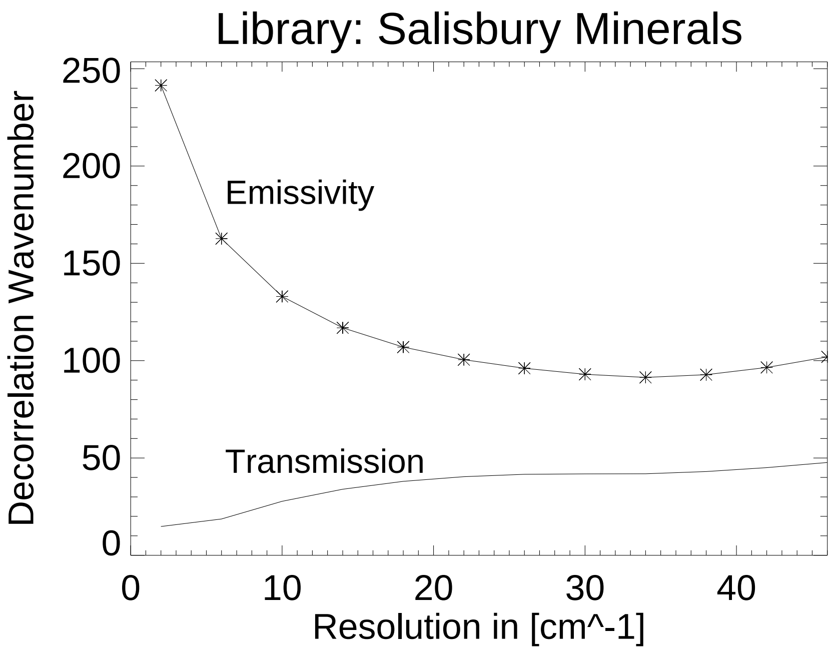
Boxcar filter filters transmission and emissivities:

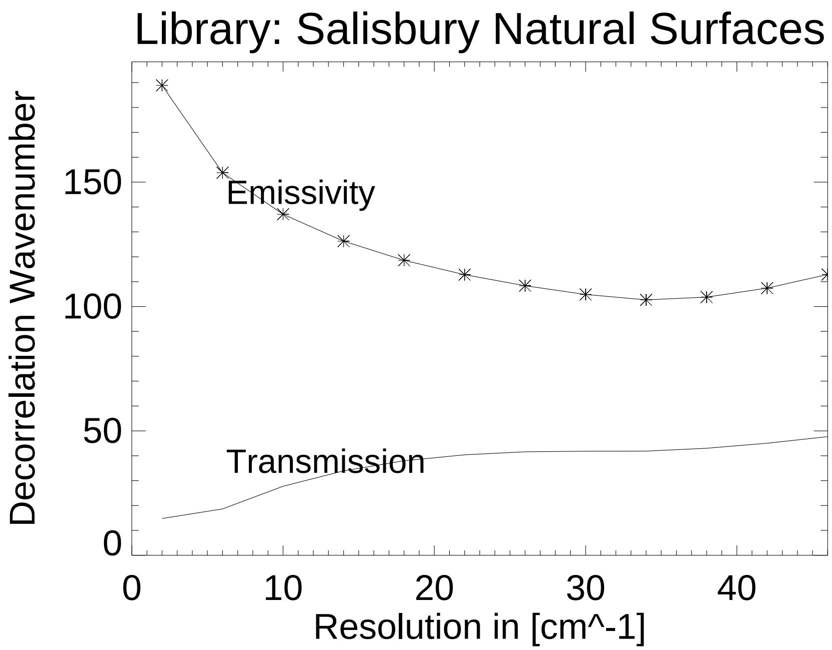
$$x_{k,W} = \frac{1}{W} \sum_{k=0}^{W-1} x_{k+j-W/2}, k = W/2, ..., N - W/2. \tag{5}$$

Autocorrelation as a function of sensor resolution in cm^{-1}



Decorrelation as a function of sensor resolution in cm^{-1}





Result:

The decorrelation wavenumber for the emissivities is more than 100 cm^{-1} and almost constant for resolutions of 10 cm^{-1} or greater. $\Rightarrow$ need at least a resolution of 10 cm^{-1} or better to distinguish atmospheric spectral features from emissivity features.

Algorithm with Variable Emissivity: ASSETR-$\delta\varepsilon$

Assumptions for ASSETR:

- Perfect sensor (no spectral and radiometric errors),
- Spectral range in the TIR from 7.5 to 13.9 μm with 100 or more spectral channels
- The atmosphere is assumed to have the transmission and path radiances of a US standard atmosphere with a thin cirrus cover.
- The flight altitude was set to 3.7 km with a surface at 1.31 km above sea level.
- No mixed pixels - one material and temperature per pixel.

Steps (short version):

1. Compute the blackbody temperature T_{bb} in an atmospheric window from an atmospherically corrected radiance L_{cor}.
2. Compute spectral emissivity: $\varepsilon = L_{cor}/B(\lambda, T_{bb})$
3. Try out different emissivity offsets $\delta\varepsilon$ and recompute ε iteratively.
4. Stop iteration when emissivity is smoothest.

Steps (long version):

The following steps were used to estimate surface temperature and emissivity (note that we left the spectral dependence of most parameters):

1. Guess of a spectrally uniform emissivity, e.g. $\varepsilon(0) = 0.95.$
2. Compute a simple atmospherically corrected blackbody radiance using:

$$L_{cor}(0) = \frac{L_{total} - L_{path\uparrow} - L_{reflected}}{\varepsilon(0)\tau_{atmo}}, \tag{6}$$

   where L_{total} is the total radiance at the sensor and $L_{path\uparrow}$ is the up-welling path radiance and $-L_{reflected}$ is given by eq. (2).

3. The ratio $\varepsilon(1)$ of a atmospherically corrected blackbody radiance $(L_{cor}(0))$ over the radiance of a blackbody at the temperature $(T_{est}(0))$ computed from L_{cor} in an atmospheric window (e.g. 10.4 to 11.5 μm) is a estimate for the shape of the emissivity:

$$\varepsilon(1) = \frac{L_{cor}(0)}{B(\lambda_i, T_{est}(0))}, \tag{7}$$

   where $B(\lambda_i, T_{est}(0))$ is the blackbody radiance of a blackbody at temperature $T_{est}(0)$ at wavelength λ_i, where $T_{est}(0)$ is given by:

$$T_{est}(0) = MEAN(B^{-1}(10.4 < \lambda < 11.5\mu m, L_{cor}(0)), \tag{8}$$

   where B^{-1} is the inverse Planck function and $lambda$ is wavelength.

4. For $n = 1, ..., N$ iterations and for $m = 1, .., M$ emissivity offsets:

$$\varepsilon_{off}(m) = m\delta\varepsilon, \tag{9}$$

where $\delta\varepsilon = 1./(M-1)$ compute the atmospheric corrected blackbody ground radiance:

$$L_{cor}(n) = \frac{L_{total} - L_{path\uparrow} - L_{reflected}(n)}{\varepsilon(n, m))\tau_{atmo}}, \tag{10}$$

where $L_{reflected}(n)$ is the reflected down-welling path radiance:

$$L_{reflected}(n) = L_{path\downarrow}(1 - (\varepsilon(n, m)))\tau_{atmo}, \tag{11}$$

where $\varepsilon(n, m) = \varepsilon(0) - \varepsilon_{off}(m)$.

5. The ratio of $L_{cor}(n)$ over the radiance of a blackbody at the temperature $T_{est}(1)$ estimated in the atmospheric window region is now a differential emissivity $\Delta\varepsilon(n)$ which is added to get an updated emissivity:

$$\varepsilon(n + 1, m) = \varepsilon(n, m) + \Delta\varepsilon(n), \tag{12}$$

where $\Delta\varepsilon(n) = L_{cor}(n)/B(\lambda_i, T_{est}(n)) - 1$ is a term which approaches zero when the estimated emissivity is exactly equal to the true emissivity. $T_{est}(1)$ is calculated from:

$$T_{est}(n) = B^{-1}(10.4 < \lambda < 11.5\mu m, L_{cor}(n)). \tag{13}$$

6. The converged emissivities $\varepsilon(N,m)$, $m = 1,\ldots,M$ are now tested for smoothness by computing the standard deviation of the difference between the retrieved emissivity $\varepsilon(N,m)$ and a box-car averaged version:

$$\sigma(\varepsilon(m)) = STDEV(\varepsilon_i(N,m) - BOXCAR(\varepsilon_i(N,m),K), i = 0, ..., N \tag{14}$$

where:

$$BOXCAR(\varepsilon_i(N,m),K) = \frac{1}{K}\sum_{j=i-K/2}^{i+K/2-1}\varepsilon_j(N,m) \tag{15}$$

where K is the number of points to calculate the spectral average.

7. Repeating steps 4-6 for M emissivity offsets we pick the offset $\delta\varepsilon(m_{opt})$ with the smallest standard deviation $\sigma(\varepsilon(m_{opt}))$ as the spectrally smoothest emissivity:

$$\varepsilon_{est} = \varepsilon|_{\sigma(m_{opt})=min}. \tag{16}$$

Notes:

1. To insure physically reasonable results we limit the atmospherically corrected radiances to positive, non-zero values.
2. The emissivity shape $\varepsilon(1)$ is limited to values between 0. and 1.

Algorithm with Variable Temperature: ASSETR-δT

Steps (short version - difference to ASSETR-$\delta\varepsilon$ in green):

1. Compute the blackbody temperature T_{bb} in an atmospheric window from an atmospherically corrected radiance L_{cor}.
2. Compute spectral emissivity: $\varepsilon = L_{cor}/B(\lambda, T_{bb})$
3. Try out different temperature offsets δT and recompute ε iteratively.
4. Stop iteration when emissivity is smoothest.

Differences to ASSETR-$\delta\varepsilon$:

- Produces no emissivities above 1. or below 0.
- Implemented a version to vary cumulative water vapor amount PW and effective atmospheric temperature $T_{atm,eff}$.

Steps (long version):

1. Solve eq. (1) for ε:

$$\varepsilon = \frac{L_{total} - L_{path\uparrow}(PW) - L_{path\downarrow}\tau_{atmo}(PW)}{(B(\lambda, T_{est}(n)) - L_{path\downarrow})\tau_{atmo}(PW)}, \tag{17}$$

   where the estimated ground temperature $T_{est}(n)$ is given by:

$$T_{est}(n) = B^{-1}\left(\lambda_{window}, \frac{L_{total} - L_{path\uparrow(PW)} - L_{path\downarrow}0.05}{0.95\tau_{atmo}(PW)}\right), \tag{18}$$

   where $\lambda_{window} = 10.4 < \lambda < 11.5\mu m$. The index n denotes the iterations, e.g. $n = 0, 1, 2, 3...$ and is an index to the temperature offsets δT in step 3. Note that we neglect the dependence of $L_{path\downarrow}$ on the water vapor and atmospheric temperature for the sake of simplicity.

2. For spectral radiances over surfaces such as water were we know the emissivity do:

   (a) Approximate the up-welling path radiance by:

$$L_{path\uparrow} = B(\lambda, T_{atmo,eff})[1 - \tau_{atmo}(PW)], \tag{19}$$

   where the effective atmospheric temperature is $T_{atmo,eff}$ and the water vapor dependent atmospheric transmission is approximated by:

$$\tau_{atmo}(PW) = \tau_{no\ H_2O}10^{-\alpha_{H_2O}PW} \tag{20}$$

where the transmittance of the atmosphere without water $\tau_{no\ H_2O}$ is computed by:

$$\tau_{no\ H_2O} = \frac{\tau_{total}}{\tau_{H_2O}}, \tag{21}$$

and the water vapor absorbance $alpha_{H_2O}$:

$$\alpha_{H_2O} = -\frac{1}{PW_0} log_{10}(\tau_{H_2O}), \tag{22}$$

where PW_0 is the cumulative water vapor amount between the sensor and target using a MODTRAN standard atmosphere and PW is the new water vapor amount (e.g. $PW = 0.5, \ldots, 2$..

(b) We found it is easy to find an appropriate emissivity by repeating the previous step and first step for a number of effective atmospheric temperature (e.g. 3-20 K) and cumulative water vapor amounts until a reasonable emissivity (e.g. 0.98@$10.4\mu m$) is found.

(c) We use the best estimate of water vapor PW_{est} and atmospheric temperature $T_{atmo,est}$ to compute new up-welling path radiance and atmospheric transmission in eqs. (17) and (18) of step 1.

3. For all spectral radiances use the optimized up-welling path radiance and atmospheric transmission terms and compute the spectral emissivity $\varepsilon(\lambda)$. The temperature is varied in eq. (17) using $T_{est}(n) = T_{est}(0) - T_{range}/2 + n\delta T$, where $\delta T = T_{range}/(N-1)$ and $n = 1, \ldots, N$. For each spectral emissivity

the smoothness is computed using eq. (23) and the smoothest emissivity is chosen:

$$\sigma(\varepsilon(m)) = STDEV(\varepsilon_i(N,m) - BOXCAR(\varepsilon_i(N,m),K), i = 0,...,N \tag{23}$$

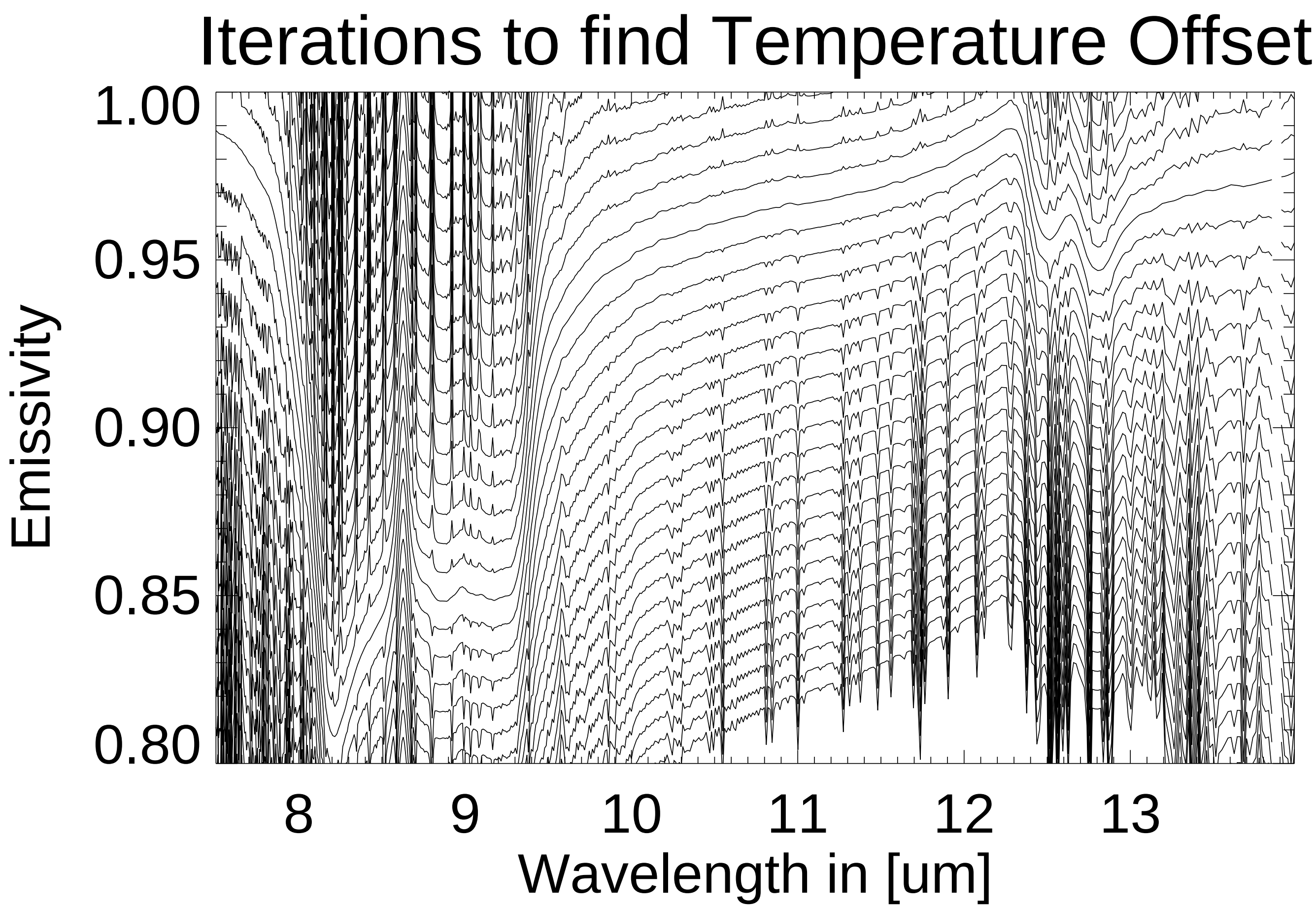
where:

$$BOXCAR(\varepsilon_i(N,m),K) = \frac{1}{K}\sum_{j=i-K/2}^{i+K/2-1} \varepsilon_j(N,m) \tag{24}$$

where K is the number of points to calculate the spectral average.

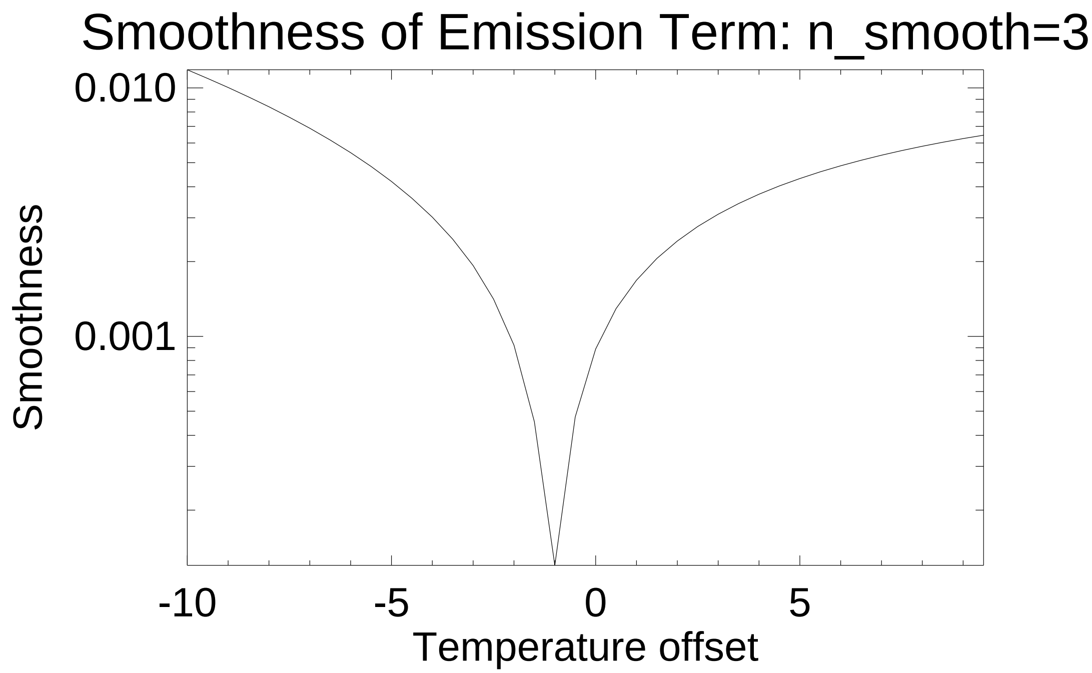
4. Thus the optimum surface temperature is then given by $T_{est,surface} = T_{est}(0) + \delta T_{min}$, where δT_{min} is the temperature offset which minimizes $\sigma(\varepsilon)$.

Retrieved emissivity as a function of temperature offset δT:



Note how important good knowledge on the atmosphere is and how narrow some of the gas absorptions are. The sampling is $1\ cm^{-1}$ and $2\ cm^{-1}$ resolution using MODTRAN3.

Emissivity smoothness as a function of surface temperature offset from the estimated ground:



Example result: true surface temperature was 290 K and the estimated temperature was 290.021. The RMS error of the emissivity in the region from 8.2 to 13 μm was 0.082.

Atmospheric Effects

Questions:

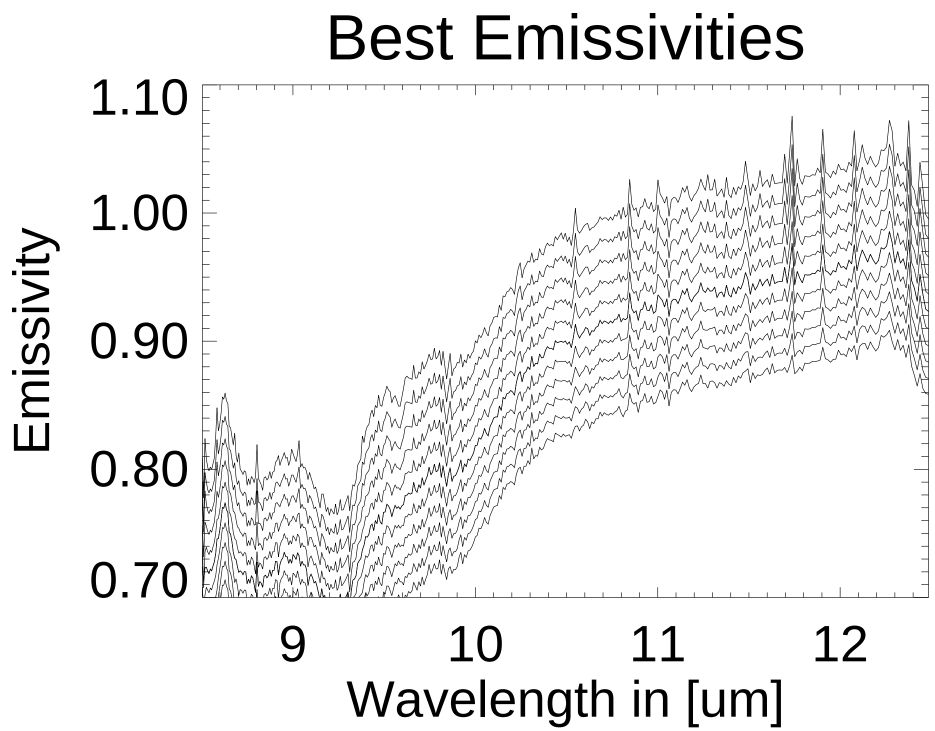
- Can we retrieve temperature and emissivity if atmospheric parameters (e.g. temperature and cumulative water vapor) are not known?
- How can the ambiguity in retrieving PW and $T_{atm,eff}$ be resolved?

Solutions: It is necessary to compute a number of emissivity solutions for the optimum combination's of PW and $T_{atm,eff}$ as a function of T_{ground} and then select the one which compares well with (i) ground truth or (ii) library spectra of known surfaces (e.g. water).

Simulation:

- The surface temperature was varied in 1 degree steps from -5 to 5 degrees around the true surface temperature and the best retrieved emissivity was plotted.
- Notice the smoothness is nearly the same but some of the emissivities are non-physical (4 curves with emissivities above 1).

Result of a retrieval (SNR=300) over a USDA soil



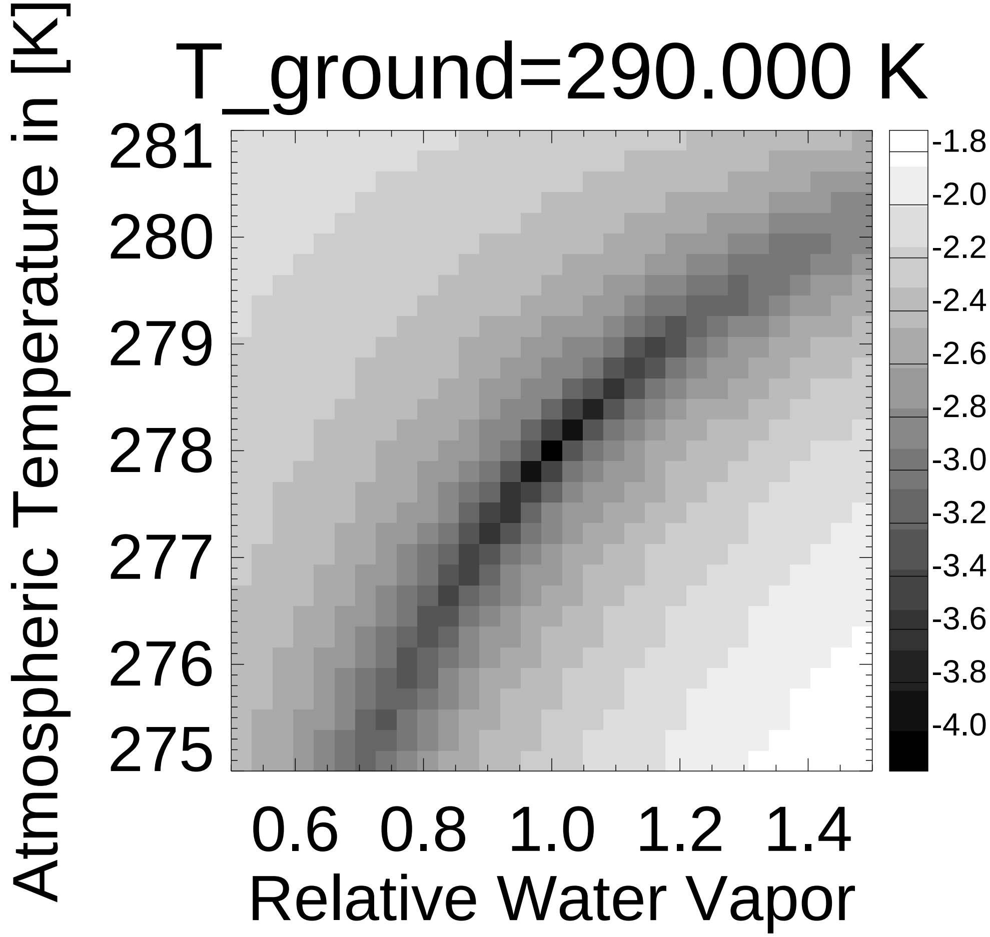
Sensitivity/Uniqueness Test:

1. Approximate the path radiance by:

$$L_{\uparrow} = B(\lambda, T_{atm})(1 - exp(-\tau(\lambda, PW))). \qquad (25)$$

2. Vary two parameters: the effective atmospheric temperature T_{atm} and the column water vapor content PW.

2D result of the smoothness as a function of atmospheric temperature T_{atm} and relative water vapor content PW/PW_0 for Salisbury: *Soil USDA 87P706*:



Discussion:

- There is a curved valley in which smooth emissivities can be retrieved.
- A sharp minimum (10^{-4} exists at $PW/PW_0 = 1$ and $T_{atm} = 278\ K$.
- Since the effective atmospheric temperature and column water vapor vary

slowly in a given scene it should be possible to retrieve PW and T_{atm} over many pixels and find the most likely combination.

- Gradient search versions of the ASSETR algorithms can be used to retrieve ε and T_{ground} very accurately (0.002 K and $\sigma_{\varepsilon} = 3.1e-5$ for 181 out of 182 Salisbury emissivities (no noise assumed). The only material which failed was *Chiastolic Slate H&S 462*, a very high emissivity ($\overline{\varepsilon} = 0.976$) material with a variance of only .6 %.

- To make the gradient search find the true optimum it was sometimes necessary to start from several initial guesses for the surface temperature based on a series of assumed spectrally constant emissivities (e.g. $\varepsilon(0)$ =0.99, 0.96, 0.93,...).

Review of Maximum-Minimum Difference (MMD)

[Matsunaga, 1993; Gillespie et al., 1996]

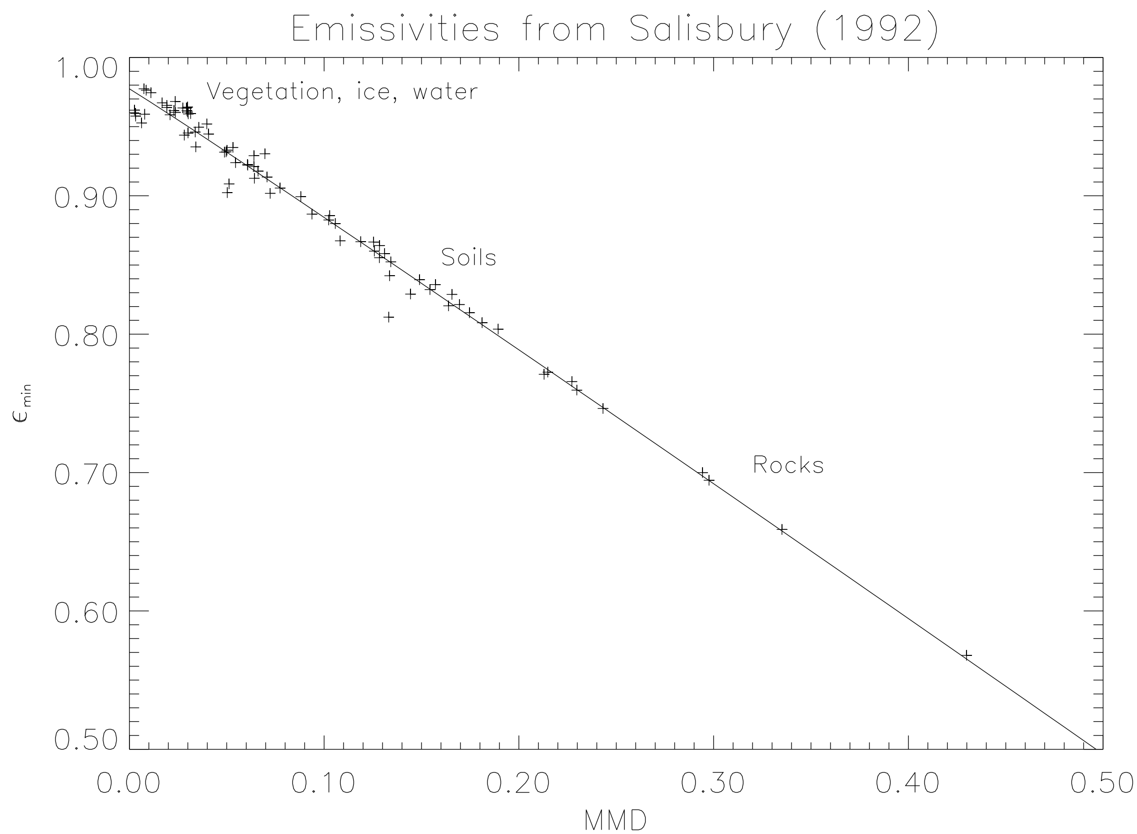
Steps:

1. Compute spectral contrast or MMD.
2. Use empirical relationship to find minimum emissivity ε_{mmd}.
3. Shift emissivity so that $min(\varepsilon(\lambda)) = \varepsilon_{mmd}$.

Empirical relation ship for Salisbury natural surface emissivities:

$$\epsilon_{mmd} = 0.997 - 0.976 * MMD^{1.02}$$

.



Empirical relationship between the minimum emissivity value for 80 natural materials in the spectrum and the spectral contrast, quantified as the difference between the minimum and maximum values, or "MMD."

Conclusions

- Hyperspectral sensors with 100 or more channels have the potential to simultaneously retrieve temperature, emissivities and atmospheric parameters.
- A new method has been developed which uses the smoothness of the spectral emissivity to retrieve temperature and emissivity.
- A good atmospheric correction is a necessary condition to retrieve accurate surface temperatures and emissivities.

Future Work

- Need to perform a sensitivity study to investigate the effect due to calibration errors (spectral and radiometric) and sensor noise.
- Investigate potential of using smoothness for in-flight spectral calibration.
- Need to investigate problem of mixed pixels on ASSETR.
- Investigate the use of low-emissivity surfaces to retrieve down-welling path radiances.
- Compare ASSETR to other methods, e.g. MMD.

Acknowledgments:

Many fruitful discussions with Dr. Bradley G. Henderson, Dr. Steve Love and Dr. William Clodius - all in NIS-2, LANL.

References

- Gillespie, A. R., S. Rokugawa, S. J. Hook, T. Matsunaga, and A. B. Kahle, Algorithm theoretical basis document for temperature/emissivity separation, Version 2.3, 16 August 1996.
- Matsunaga, T., An emissivity-temperature separation technique based on an empirical relationship between mean and range of spectral emissivity, *Proc. 14th Japanese Conf. of Remote Sensing*, 47-48, 1993.
- Salisbury, J. W. and D. M. D'Aria, Emissivity of terrestrial materials in the 8-14 μm atmospheric window, *Remote Sens. Environ., 42*, 83-106, 1992.